Simulation of the production of isoamyl acetate from isoamyl alcohol obtained from fusel oil distillation.

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Isoamyl acetate is a high-valued ester widely used as a source of banana flavour by the food industry. It is commonly obtained by esterification of isoamyl alcohol with acetic acid. Isoamyl alcohol can be obtained from distillation of fusel oil, a by-product from the bioethanol industry, and can be used as “green solvent”. Thus, this work aimed to study the industrial process to obtain isoamyl acetate from fusel oil using Aspen Plus simulator. Samples of fusel oil collected in Brazilian industrial mills were analyzed by gas chromatography in order to characterize this mixture. One configuration for the purification process of fusel oil to obtain isoamyl alcohol was proposed, and some operational and constructive parameters were defined using factorial design. This configuration resulted in a recovery of 99.5 % of isoamyl alcohol with 81.8 % of purity. Isoamyl alcohol recovered from fusel oil was used with acetic acid to simulate the esterification reaction. The rate of conversion of isoamyl alcohol to isoamyl acetate through simple chemical reactions is very low and thus the use of a catalyst is required. Literature data of this esterification reaction were used to design the reactor and a good conversion was found. The results indicate that fusel oil can be used successfully as source of isoamyl alcohol and the catalyzed esterification of this alcohol with acetic acid achieves high conversion of isoamyl acetate.